

3,3'-Dichlorobenzidine
91-94-1 | DTXSID6020432

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1680 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.80e-01

Confidence level: 4.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3,3'-Dichlorobenzidine</div> <div>Measured: 22400</div> <div>Predicted: 1680</div>	<div>Image not found</div> <div>Ethyl 1-naphthaleneacetate</div> <div>Measured: 302</div> <div>Predicted: 425</div>	<div>Image not found</div> <div>Bendiocarb</div> <div>Measured: 562</div> <div>Predicted: 247</div>
<div>Image not found</div> <div>Carboxin</div> <div>Measured: 257</div> <div>Predicted: 210</div>	<div>Image not found</div> <div>Carbofuran</div> <div>Measured: 56.2</div> <div>Predicted: 110</div>	